On Using Approximations in Engineering Optimization

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Outline

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  - **Motivation**
  - **Some Recent Developments in Approximations for Engineering**
- **Model Trust-Region Approach with General Approximations**
  - **The Model-Management Framework**
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- **Current Research**
  - **Constraints and MDO**
  - **Novel Applications (HSCT, Aerospike, Rotorcraft)**
- **Summary**

Approximations-in-Optimization Problem

- **The problem:**

$$\text{minimize } f(x)$$

The essential problem is multidisciplinary and has special structure, but here will consider single discipline, unconstrained optimization.

- **Motivation**
  - Address computational expense issues of using high-fidelity approximation models in optimization (Example: Navier-Stokes vs. Euler)
  - Allow for easier integration of disciplines in multidisciplinary context
  - Allow for interactive design
- **Some history**
  - Schmit, et al. - First explicit coupling of structural analysis and nonlinear programming (1960); Some approximation concepts for structural synthesis (1960)
  - Fleury, et al. (1989) - Approximation strategies in structural optimization (analysis)
  - Barthelemy, et al. (1993) - Overview of approximation concepts in structural design
  - . . .

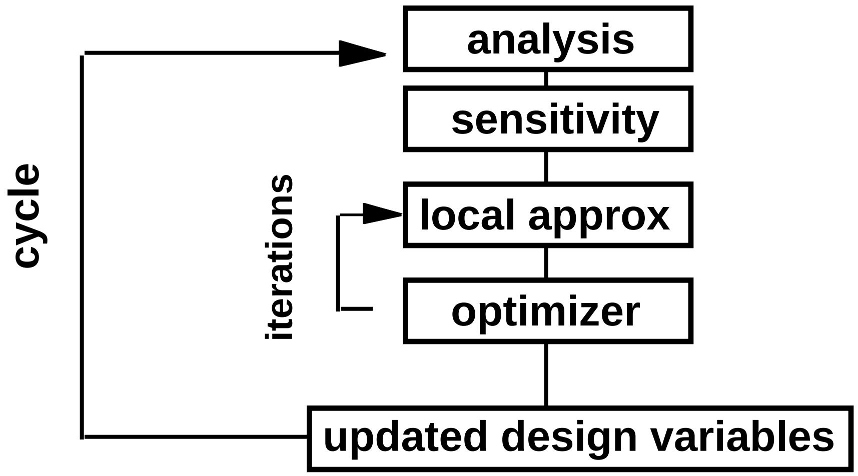
Approximations-in-Optimization Problem (cont.)

- **Existing practices**
  - Use a variety of fidelities for models or approximations managed via heuristics
  - Examples: physical models, statistical models, move limits

- **Difficulties with heuristics**
  - There is no guarantee that a design that promises improvement with a low-fidelity system will yield improvement in the high-fidelity system
  - It is not clear when to refine the model
  - Robustness is not assured

Existing Practices: Example

Optimizer and approximate analysis optimization scheme for HSCT (Walsh, et al.)



- **Evaluate objective, constraints, and derivatives of objectives and constraints at the beginning of cycle; f_0 is a coupled Navier-Stokes and finite-element analysis**

- **During optimization iterations,**

  do ...

  call optimizer with $f \approx f_0 + \sum \partial f_0/\partial x \;\; \Delta x$ (similarly for constraints g)

  + move limits

  end do

Some Recent Developments in Engineering Approximations

- Research conducted or supported at NASA Langley:
  - Design-oriented analysis and approximations
    - E. g., at University of Florida / Virginia Tech (Haftka, et al.)

      (Response Surface Approximations in High-dimensional Spaces Using Several Levels of Fidelity)
  - Approximation / modeling validation
    - E. g., at MIT / NASA Langley (Otto, et al.)

      (Computer Simulation Surrogates for Numerical Simulations and Optimization; Surrogate Pareto Approach to Shape Optimization)
  - Managing approximation models in optimization
    - E. g., at NASA Langley / ICASE;

      Notre Dame / Virginia Tech (Rodriguez, et al.)

      (Augmented Lagrangian Response Surface Approximations - Model Management Framework for General Constrained Optimization)
- Links to detailed information provided at:

  http://fmad-www.larc.nasa.gov/mdob

A Trust-Region Framework for Managing the Use of Approximation Models in Optimization

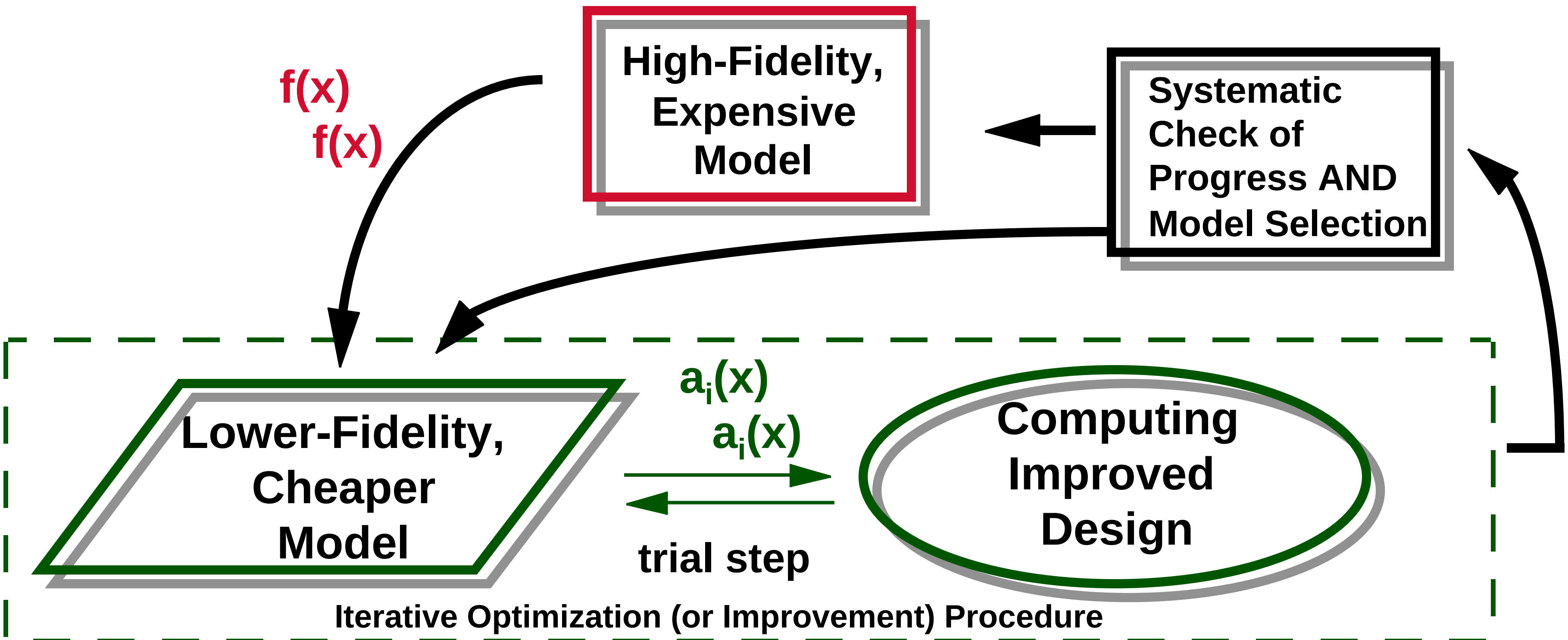
(Results by Alexandrov, et al. in *Journal on Structural Optimization*)

- **This research considers general first order approximations and answers the question "How does one make an approximation scheme robust", in particular:**
  - **What does one do when the design derived with a lower-fidelity model fails to produce improvement in the true objective?**
  - **How does one use information about the predictive value of an approximation to adjust the amount of optimization with a lower-fidelity model before recourse to the higher-fidelity model?**
  - **How does one use approximations to yield an answer to the high-fidelity problem?**
- **Observation:**
  - **The framework provides a method for managing the use of models of varying physical fidelity**

Model Trust-Region Approach with General Approximations

f(x) - high fidelity, expensive model, such as analysis or simulation

$a_i(x)$ - one of the suite of lower fidelity or accuracy models of the same physical process



Requirements on the Approximation Model

- **At each major point x_k, the following model consistency conditions are assumed to hold:**

$$a_k(x_k) = f\,(x_k)$$
$$a_k(x_k) = \quad f(x_k)$$

- **Observations:**
  - **Consistency is only enforced at the “anchor” points.**
  - **The gradients do not have to match exactly, but that is the assumption made in the published paper**

Requirements on the Approximation Model:
Enforcing the Consistency Conditions

- **In practice, consistency is an application dependent question, but there exist methods for enforcing consistency.**
- **Example: Correction by β-correlation approach. Chang et al. (1993)**

Assuming no specific functional form, let f_{lo} be a model of lower fidelity than f. Define

$$\beta(x) = \frac{f(x)}{f_{lo}(x)}$$

Given x_k, build

$$\beta_k(x) = \beta(x_k) + \quad \beta(x_k)^T (x - x_k)$$

Use β_k to scale the lower-fidelity model f_{lo}:

$$f(x) = \beta(x)\, a(x) \approx \beta_k(x)\, f_{lo}(x)$$

Then

$$a_k(x) = \beta_k(x)\, f_{lo}(x)$$

satisfies the consistency conditions.

The Algorithm with General Approximations

Choose $x_0 \quad R^n$, $\Delta_0 > 0$

For $k = 0, 1, \ldots$ until convergence do

Choose a_k such that $a_k(x_k) = f\,(x_k)$ and $a_{\,k}(x_k) = \quad f\,(x_k)$

Compute an approximate solution s_k to subproblem:

$$\begin{aligned} &\text{minimize } a_k(x_k + s) \\ &\text{subject to } \quad \|s\| \le \Delta_k \end{aligned}$$

Compare the actual and predicted decrease in f:

$$r = \frac{f\,(x_k) - f\,(x_k+s_k)}{f\,(x_k) - a_k(x_k+s_k)}$$

$$x_{k+1} = \begin{cases} x_k + s_k \text{ if } f(x_k + s_k) < f(x_k) \\ x_k \quad \text{otherwise} \end{cases} \qquad \text{and} \qquad \Delta_{k+1} = \begin{cases} c_1 \|s_k\| \text{ if } r < r_1 \\ \min\{c_2 \|s_k\|, \Delta_{max}\} \text{ if } r > r_2 \\ \|s_k\| \quad \text{otherwise} \end{cases}$$

for some $r_1 < r_2 < 1$, $c_1 < 1$, $c_2 > 1$

end do

Convergence Analysis

- **Observations:**
  - **Practical performance will depend on the quality of the approximation models and their ability to predict the behavior of f.**
  - **Options in case of unsuccessful step:**
    - **Improve model fidelity**
    - **Do less optimization - reduce the trust-region radius.**

- **Convergence:**
  - **We solve approximately:**

$$\text{minimize } a_k\,(x_k + s)$$
$$\text{subject to } \|s\| \leq \Delta_k$$

  with a_k - a general 1st order model.

  - **"Approximately" = s_k must satisfy Fraction of Cauchy Decrease (FCD). Use the variant: there exist β, C > 0, independent of k, such that s_k satisfies**

$$f(x_k) - q_k(x_k + s_k) \geq \beta \,\|\;\; f(x)\|\, \min\,(\Delta_k, \|\;\; f(x_k)\|/C).$$

  - **The following algorithm for solving the subproblem satisfies FCD:**

Computing an approximate solution s_k

Given $x_k \quad R^n$, $\Delta_k > 0$, choose $\tau \quad (0,1)$, a_1, $a_2 > 0$ and set $y_0 = x_k$, $\delta_0 = \tau\Delta_k$, $v_0 = 0$.

For $j = 0, 1, \ldots,$ until $\alpha_1\Delta_k \leq ||v_j|| < \alpha_2\Delta_k$ do

Find an approximate solution p_j to:

$$\text{minimize } q_j(y_j + p) = a_k(y_j) + \quad a_k(y_j)^T p + 1/2\, p^T H_j\, p$$

$$\text{subject to } ||p|| \leq \delta_j$$

$$||y_j + p|| \leq \Delta_k$$

that satisfies FCD for a_k from y_j.

Compare the actual and predicted decrease in a_k:

$$r = \frac{a_k(y_j) - a_k(y_j + p_j)}{a_k(y_j) - q_j(y_j + p_j)}$$

Update y_j as indicated below, update δ_j as Δ_k

$v_{j+1} = v_j + (y_{j+1} - y_j)$

end do

Set $s_k = v_j$

Updating y_j: choose $\mu > 0$, independent of k, j, and set

If $y_j = x_k$, then $y_{j+1} = \begin{cases} y_j + p_j & \text{if } r > \mu \\ y_j & \text{otherwise} \end{cases}$

If $y_j \neq x_k$, then $y_{j+1} = \begin{cases} y_j + p_j & \text{if } r > 0 \\ y_j & \text{otherwise} \end{cases}$

Convergence Analysis

- **The subproblem is itself a TR subproblem**

$$\textbf{minimize } q_j\,(y_j + p) = a_k(y_j) + \quad a_k(y_j)^T p + 1/2\; p^T H_j\, p$$

$$\textbf{subject to } \|p\| \le \delta_j$$

$$\|y_j + p\| \le \Delta_k$$

- **Exact and approximate solutions are given in Heinkenschloss (1994).**
- **Let p_N be the first acceptable step. It satisfies FCD for a_k at x_k and since r > μ,**

$$a_k(x_k) - a_k(x_k + p_N) \ge \mu\beta \,\|\quad a_k(x_k)\|\, \min\,(\delta_N, \|\quad a_k(x_k)\|/C)$$

- **Applying the consistency conditions and assuming uniform boundedness in k of Hessians $\quad^2 a_k(x+s)$ for all s with $\|s\| \le \Delta_k$ (the latter guarantees the existence of γ, independent of k for which $\delta_N \ge \gamma\Delta_k$) yields:**

$$f(x_k) - a_k(x_k + p_N) \ge \gamma\mu\beta \,\|\quad f(x_k)\|\, \min\,(\Delta_k, \|\quad f(x_k)\|/C).$$

Convergence Analysis

- Since any steps after N decrease a_k further, the step produces FCD for a_k as an approximation of f at x_k and Powell's global convergence theorem (1975) is applicable:
    - If f is uniformly bounded below, uniformly continuously differentiable, and the Hessian approximations are uniformly bounded, then the sequence of iterates generated by a trust-region algorithm whose steps satisfy FCD satisfies

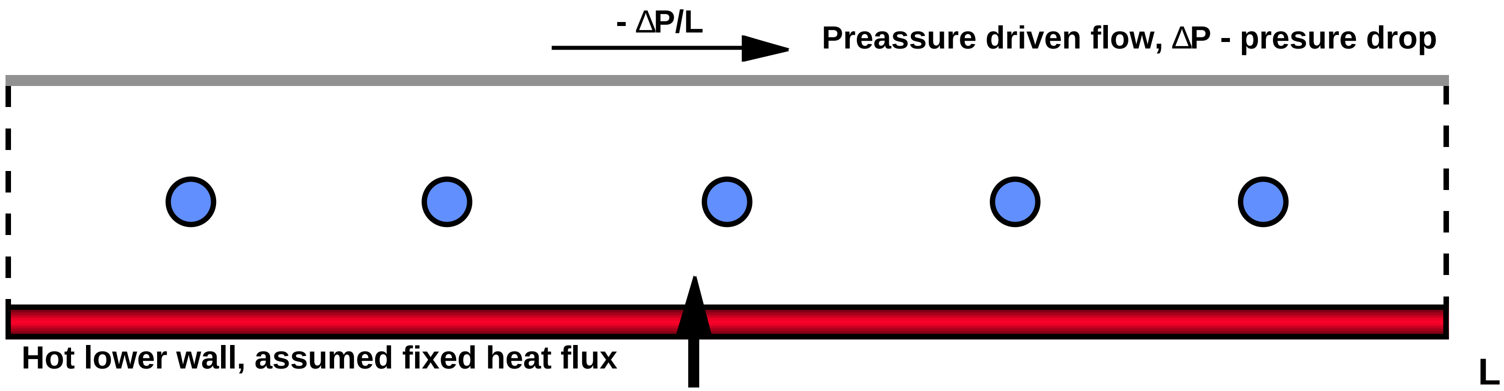
$$\liminf_{k \to \infty} \| \ f(x_k)\| = 0$$

- The use of the acceptance criterion for y_j further guarantees that

$$\lim_{k \to \infty} \| \ f(x_k)\| = 0$$

Illustrative Example

“Eddy-Promoter” Heat Exchanger (analyses / codes by Otto et al.)



- **Goal**
  - Transfer heat from the lower surface into the fluid medium as efficiently as possible
- **Objectives**
  - Lower wall temperature
  - Lower preassure gradient
- **Eddy-Promoter Configuration**
  - Periodic array of cylindrical obstructions
  - Lowers critical parameter for onset of instability
  - Improved heat transport
- **Governing Equations**
  - 2-D incompressible Navier-Stokes

Place holder

Representative problem from:

"A Surrogate-Pareto Approach to Shape Optimization: Level Set Geometry Description" by John C. Otto

Presented at the ICASE/LaRC Approximation Meeting

July 21---23, 1997

Illustrative Example (cont.)

Preliminary Results on 1st Order Model Management

- **Preliminary results on first-order model management**
  - **Assumptions**
    - **Model single periodicity cell (with doublets)**
    - **For initial computation, use fixed weights for the objectives**
    - **Use reduced problem (≈ 2 min. / N-S analysis)**
  - **One function evaluation**
    - **(at k=0, provide an initial point (3 or 6 variables))**
    - **Generate a grid**
    - **Input grid to the N-S code to generate the values of f_1 and f_2**
  - **Other ...**
    - **Derivatives are computed via finite differences**
    - **Lower-fidelity model is assumed to be a model with a coarser grid**
  - **Preliminary impression**
    - **Promising results for the chosen models**

Current Research: Constraints and MDO

- **Equality Constraints**
  - Extension of the 1st order model management framework via the multilevel algorithm for equality constrained optimization (Alexandrov, 1993)
  - Global convergence results (Alexandrov, 1997)
- **General NLP**
  - Based on Alexandrov-El-Alem extension to general NLP of the multilevel algorithm for equality constrained optimization
- **MDO**
  - Many research questions, dependent on problem formulations

Current Research: Some Novel Applications at MDOB

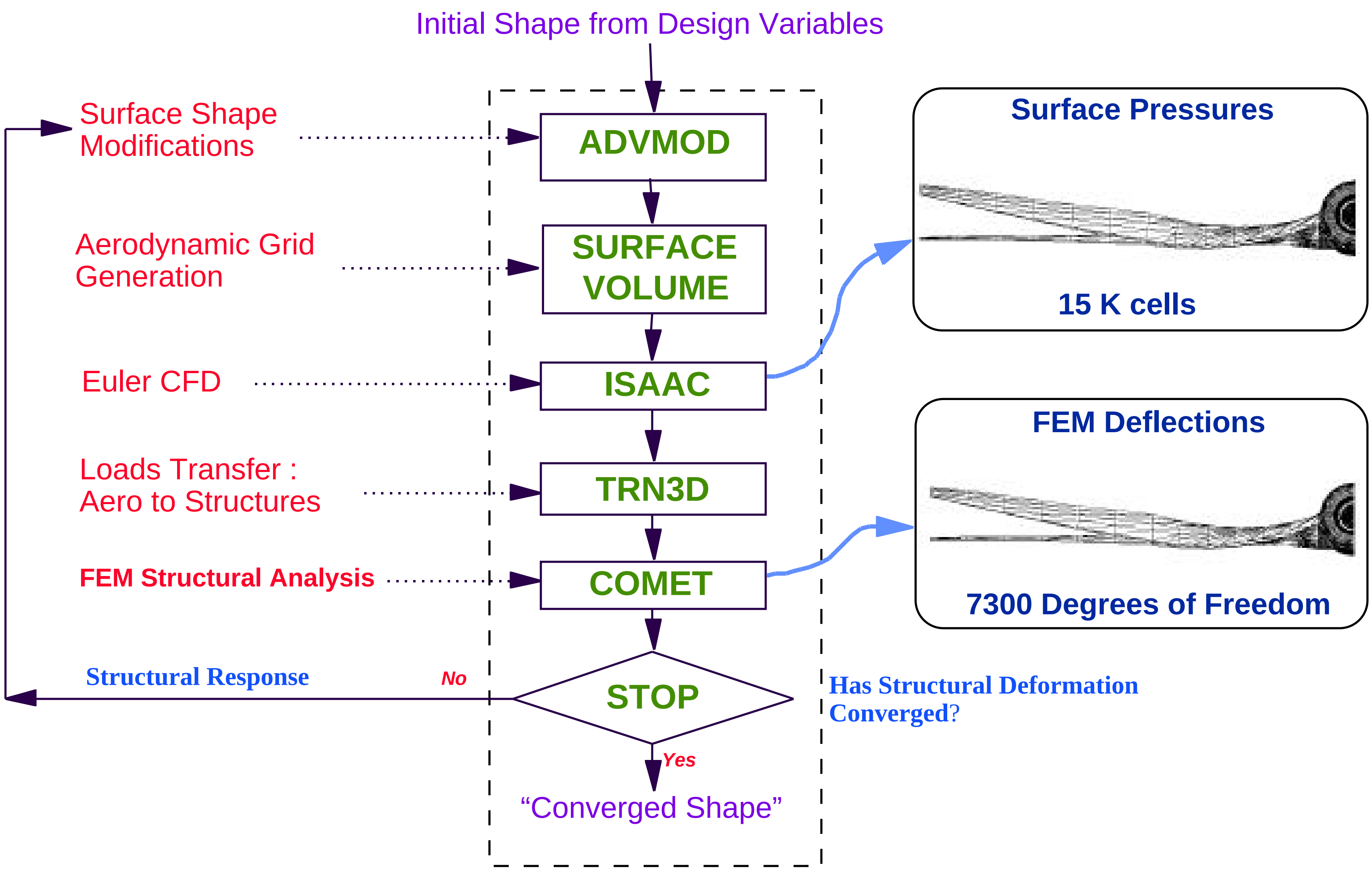
- **Applications**
  - High Speed Civil Transport (HSCT)
  - Aerospike Nozzle Design for RLV Concepts
  - Rotorcraft Blade Design

- **Common features:**
  - When used in high-fidelity mode
    - Large number of variables and constraints
    - Computationally expensive
    - Interest in using both statistical approximations and lower-fidelity physical approximations

Novel Applications: HPCCP HSCT
(Weston, et al.)

- **Problem Features:**
  - **Components:**
    - **Multiblock Navier-Stokes CFD analysis & sensitivity**
    - **Adaptive FEM structural analysis & sensitivity**
    - **Many other disciplines**
  - **Computationally intensive:**
    - **Medium-fidelity**
      - **One aeroelastic function evaluation (multidisciplinary analysis of ≈ 5 Gauss-Seidel iterations) requires 6 hours on a heterogeneous network of 4-5 machines; ≈ 20 hours on a dedicated machine**
    - **High-fidelity**
      - **One aeroelastic function evaluation is expected to require 5-6 days on a dedicated machine; 2 days on a parallel machine; 3-6 hours on 64-processor machine ($O(10^2)$ hours total)**

Novel Applications: HSCT - Key Steps



Novel Applications: Rotorcraft Blade Optimization
(Walsh, et al.)

- **Problem Features:**
  - Large number of design variables and constraints
  - A multilevel approach to solution
  - Computationally intensive
    - One function evaluation requires ≈ 30 minutes

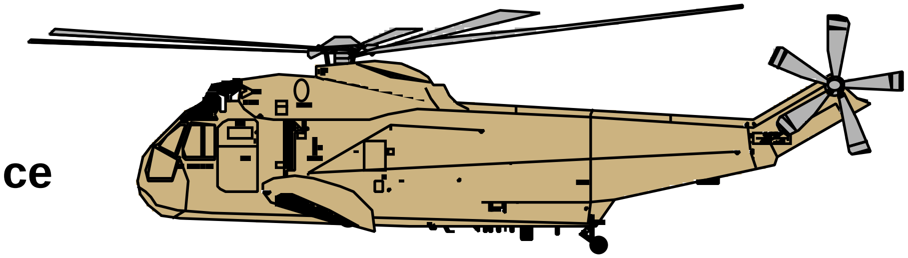
Integrated Aerodynamic/Dynamic/Structural (IADS) Solution Strategy

Optimize for global behavior
(aerodynamics, dynamics, strains)

Optimize cross section radial location 1	Optimize cross section radial location 2	Optimize cross section radial location 3

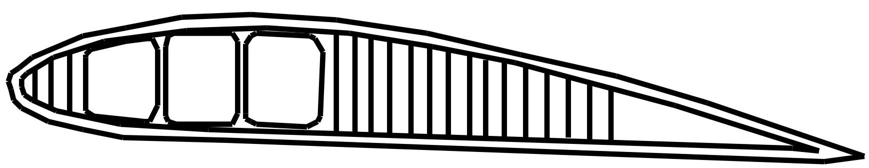
Integrated Aerodynamics/Dynamics/Structures (IADS)

<u>UPPER LEVEL</u>:
optimize performance and dynamics



Compromise between stiffness required by upper level and attainable in lower level

<u>LOWER LEVEL</u>:
design internal structure at radial location i

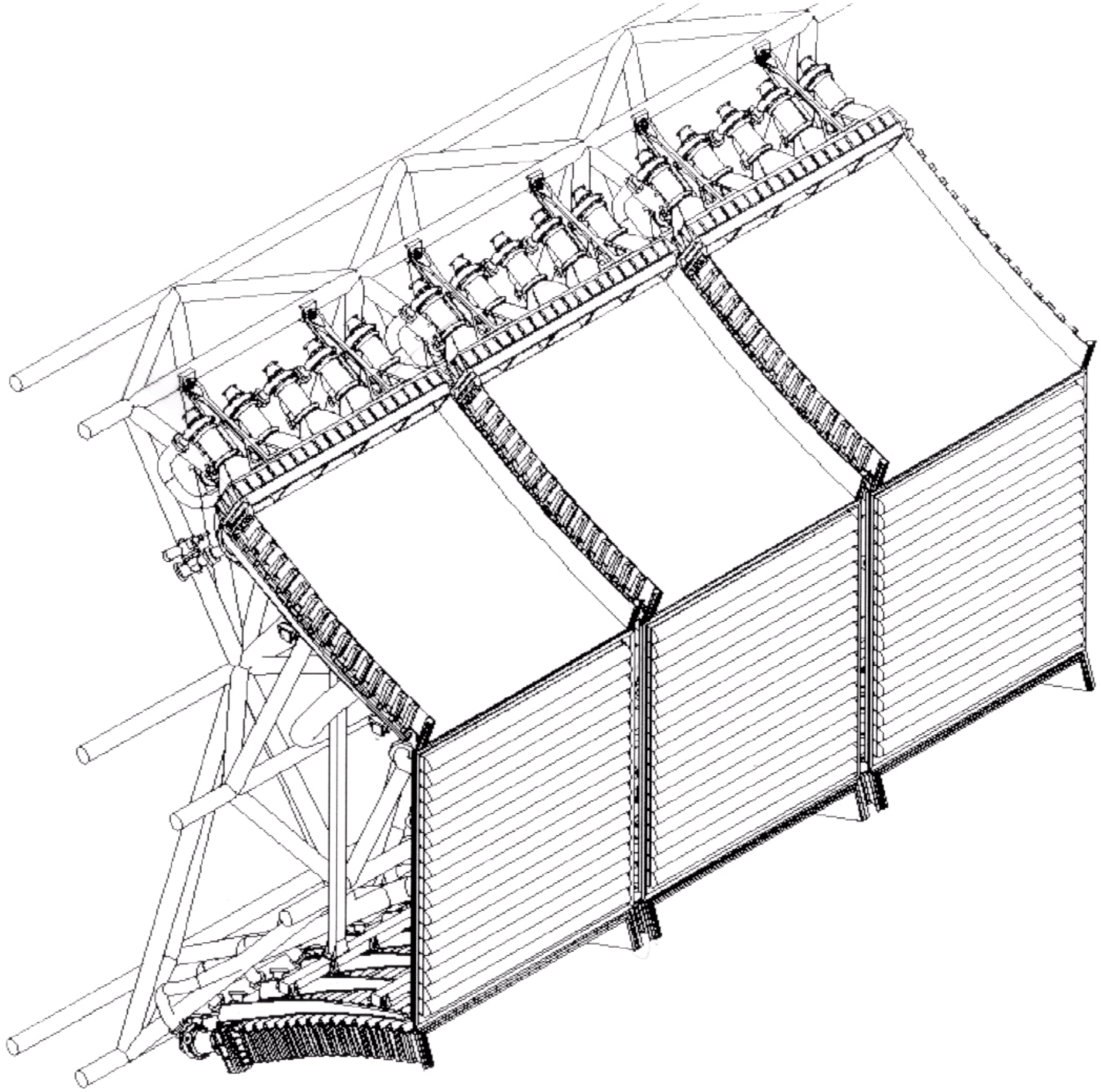


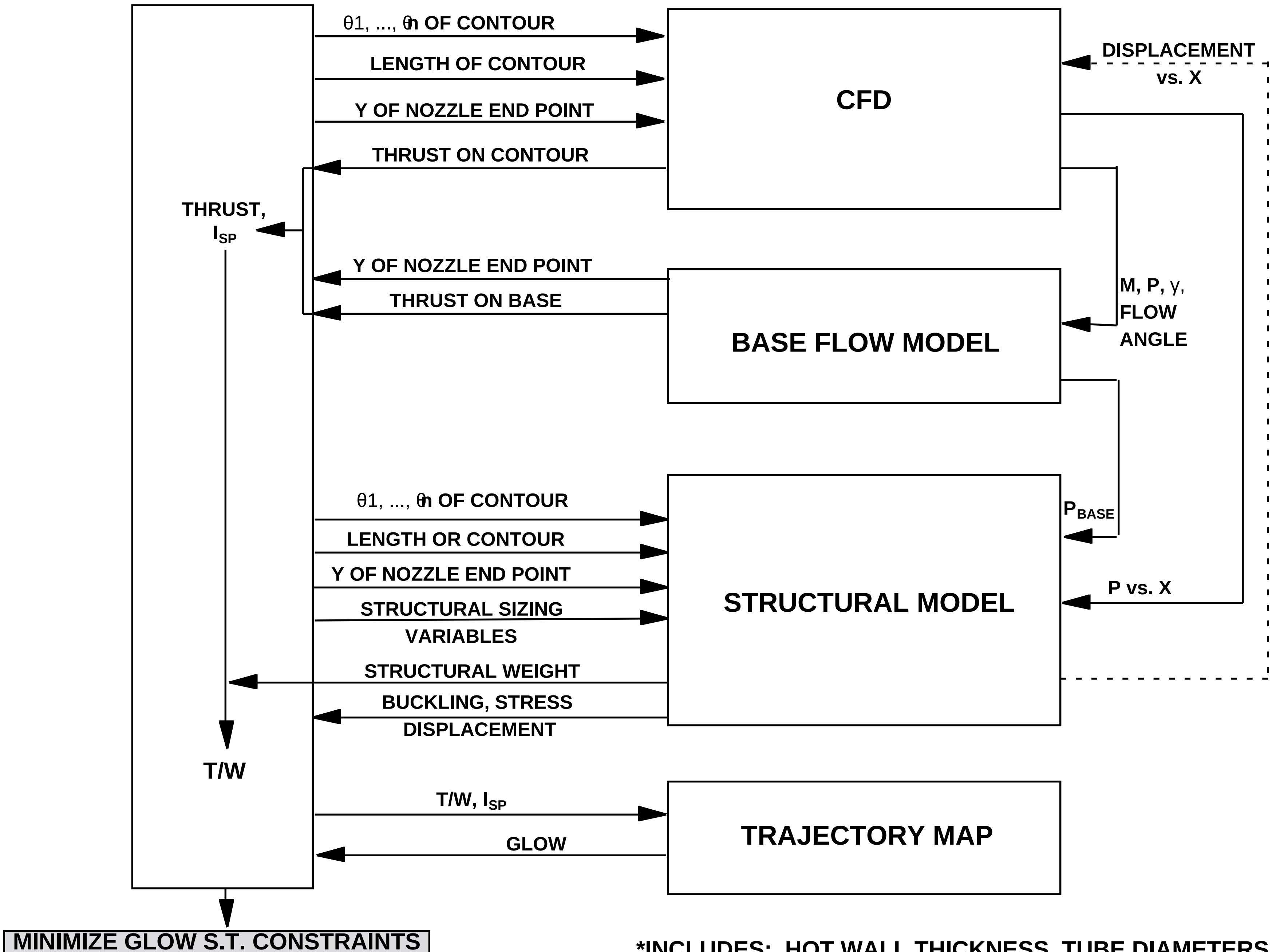
Novel Applications: Aerospike Engine Design
(Korte, et al.)

- **Problem Features:**
  - **Components:**
    - **Aerodynamics, structures, trajectory**
    - **High accuracy required due to sensitivity of SSTO vehicle performance**
    - **Minimize GLOW (Gross Lift-Off Weight) subject to structural constraints**
    - **One case: 16 variables, 596 structural constraints**
    - **Multidisciplinary feasible formulation used**
  - **Computationally intensive**
    - **Low-fidelity**
    - **Medium-Fidelity**
    - **High-fidelity**

RLV X-33 Concepts

AEROSPIKE ENGINE





*INCLUDES: HOT WALL THICKNESS, TUBE DIAMETERS, TUBE WALL THICKNESS, I-BEAM WEB THICKNESS, ET.

Summary

- Extensive, long-standing research on approximations in engineering optimization
- Benefit of research on approximations
  - An opportunity to adapt state-of-the-art optimization algorithms to practical computational engineering
- Introduced a framework for managing 1st order models in optimization
  - Globally convergent
  - Arbitrary models with consistency requirements
- Ongoing research - open questions:
  - Usefulness in practice
    - Testing on increasingly realistic problems
    - Resolving consistency conditions in practice
  - MDO